

Peter Egelstaff: some Happy Memories

I clearly recollect my first meeting with Peter. At dinner in St John's College in 1963 he was the guest of Roger Elliott and was working on the scattering from liquid hydrogen at low temperatures. Particularly interested then in para-hydrogen he said to me (a new Fellow in Chemistry at St John's College) – “you're a chemist so you must know all about *ortho* and *para* hydrogen....”. There began a long conversation and the beginnings of my interaction with him and, for me, of my experience of neutron scattering. I had developed an interest in particle scattering and molecular beams as a new scientific interest on getting my Fellowship but Peter's enthusiastic advocacy of the all-comprehensive content of the “neutron scattering law” drew me away.

Within weeks I had visited him in building 436 at Harwell and began to understand the spectroscopic potential of cold neutron scattering, appreciating also his great achievement of making a cold neutron source and spectrometer in the DIDO reactor at Harwell. I began also to appreciate the scientists and technicians gathered around him and the many good conversations down at the end of the corridor with him in his office. My first student Julia Higgins and I began work on neutron scattering from molecular substances looking for molecular excitations with incoherent scattering. I saw that the scattering law had to be simplified by using isotopic or atomic contrast to distinguish molecular excitations within the overall scattering. An interest at that time in localised modes led to our first paper with him on the dynamics of trapped molecules inside quinol clathrates - where the host material was fully deuterated (by Julia) allowing contrast to it for the hydrogenous trapped molecules [1].

In the same vein with Peter, we published the first paper on trapped molecules in zeolite catalytic materials- of industrial interest [2]. John Hall and others in Peter's group solved the multi-angle data acquisition problem from the detector bank on the 4H5 instrument on DIDO - the “event mode” data being recorded on a television video recorder – to be played back at high speed into John Hall's “Cassandra” PDP-8 computer for analysis. (There was not only the lower counter bank on 4H5 but another above - with solid state detectors - for Gordon Squires and his students David Price, Roger Pynn and Sunil Sinha recording collective excitations in solids and benefiting in the same way.)

Peter's drive and enthusiasm had brought all of this together as a working instrument used by him for the ground-breaking work on simple and molecular liquids and by us for molecular spectroscopy – eventually using deuterium substitution with my students Aldred and Eden to try to separate the picosecond motions of different parts chemical groups in a molecular liquid [3]. With Peter there was never any suggestion that things wouldn't work – some way would be found theoretically or experimentally. In those early days of scattering his bright-eyed confidence and the encouragement to my students, as they wrote programs for data refinement and interpretation, was inclusive and highly appreciated.

It was decided that a new instrument would be built to meet the increasing demand for time on 4H5. This was the 6H machine, which George Stirling, George Haines and Harwell engineers designed with great accuracy. The detector bank had equal length flight paths at precise distances from the sample and led us to overcome the first Egelstaff-White law of neutron scattering [4] that “all neutron spectra are the same”. The sharp molecular excitations were seen also on 4H5 after the new cold source was put in to that hole especially during the “supernova” period before it failed. It is just as well we had 6H to carry on with, as at that time Tom Waddington and Geoffrey Allen were coming into the chemical neutron scattering business. We had a discussion about the counter banks and how big they could be – counting rates were always slow and Peter came up with an idea on paper as we discussed it in his office - the DDD (Diffractionists’ Dream Detector). This was a cylindrical structure with counters covering the inside surface and the beam entering horizontally in the middle of the cylinder. On finishing the drawing, he gave the characteristic Egelstaff chuckle, half believing, half doubting that such a thing could be made – but with the conviction that it should be made.

Peter’s Academic Press “Neutron Scattering” with chapters by expert colleagues showed the scope of the method in the science of materials and his little book on liquids became highly appreciated and the basis of a graduate lecture course that I gave at Oxford. The late 60s and early 70s were the heyday of analytic models for the scattering function, for lattice dynamics of crystals and the beginning of molecular dynamic simulations for liquids. The instrumentation and theory that he developed and his background in particle physics and the work of the solid state division at Harwell including Mick Lomer, Walter Marshall and Peter Schofield, to name a few, underpinned neutron scattering for many years to come. A minor but persistent legacy is **Q** for the scattering vector.

John White

Research School of Chemistry, Australian National University, Canberra ACT 0200

3-Feb-2015

References

1. Downes, J. S., Egelstaff, P. A., Rainey, V. and White, J. W. – Localized Vibrations of Trapped Molecules. *Phys. Rev. Lett.*, 17: pp. 533–536 (1966).
2. Egelstaff, P. A., Stretton Downes, J. and White, J. W. – Molecular Motion in Molecular Sieves by Neutron Scattering Spectroscopy. In *Molecular Sieves, Soc. of Chem. Ind.*, pp. 306–318 (1968).
3. Aldred, B. K., Eden, R. C. and White, J. W. – Neutron Scattering Spectroscopy of Liquids. *Discuss. Farad. Soc.*, 43: pp. 169–183 (1967).
4. P.A.Egelstaff in “Neutron Scattering for the Analysis of Biological Structures”. Ed B. Schoenborn, Report of a Symposium held 2-6 June 1975, BNL 50453, I-33, Biology and Medicine TID- 4500, Brookhaven National Laboratory